=> d his

(FILE 'HOME' ENTERED AT 17:20:08 ON 14 MAR 2001) FILE 'REGISTRY' ENTERED AT 17:20:11 ON 14 MAR 2001 STRUCTURE UPLOADED L1 L2 4 S L1 119 S L2 FULL L3 FILE 'CA' ENTERED AT 17:20:57 ON 14 MAR 2001 L46 S L3 L5 1 S L4 AND OHKAWA, S?/AU 5 S L4 NOT L5 L6 FILE 'REGISTRY' ENTERED AT 17:23:30 ON 14 MAR 2001 L7 STRUCTURE UPLOADED 0 S L7 L8 135 S L8 FULL L9 FILE 'CA' ENTERED AT 17:24:35 ON 14 MAR 2001 8 S L9 L10 2 S L10 NOT L4 L11FILE 'CA' ENTERED AT 17:25:21 ON 14 MAR 2001 8 S L9 L12 FILE 'CAOLD' ENTERED AT 17:25:37 ON 14 MAR 2001 L13 0 S L9 =>

---Logging off of STN---

Executing the logoff script...

=> LOG Y

SINCE FILE TOTAL COST IN U.S. DOLLARS SESSION ENTRY 0.31 303.15 FULL ESTIMATED COST SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SESSION ENTRY 0.00 -4.48 CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 17:26:03 ON 14 MAR 2001

ring/chain nodes :
 11 12
chain bonds :
 7-13
ring/chain bonds :
 8-12 8-11
ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :

5-7 6-9 7-8 7-13 8-9 8-12 8-11 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 isolated ring systems : containing 1 :

1 2 3 4 5 6 7 8 9

chain nodes :
 13 15
ring nodes :

G1:0,S G2:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:Atom 15:CLASS 16:CLASS

STN Structure : 09445193.str

```
13 15
ring nodes:
1 2 3 4 5 6 7 8 9
ring/chain nodes:
11 12
chain bonds:
7-13 8-12 8-11
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds:
5-7 6-9 7-8 7-13 8-9 8-12 8-11
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems:
containing 1:
```

G1:0,S G2:0,S

chain nodes :

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:Atom 15:CLASS 16:CLASS

Connecting via Winsock to STN

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TERMINAL (ENTER 1, 2, 3, OR ?):2

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL SESSION 0.15 0.15

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 13 MAR 2001 HIGHEST RN 327020-77-9 DICTIONARY FILE UPDATES: 13 MAR 2001 HIGHEST RN 327020-77-9

TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when conducting ${\tt SmartSELECT}$ searches.

Structure search limits have been increased. See $\ensuremath{\mathsf{HELP}}$ $\ensuremath{\mathsf{SLIMIT}}$ for details.

≔>

Uploading 09445193.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS L1 STR

G1 0, S

G2 0, S

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 17:20:44 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1213 TO ITERATE

82.4% PROCESSED 1000 ITERATIONS

4 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**
PROJECTED ITERATIONS: 22172 TO 26348
PROJECTED ANSWERS: 4 TO 229

L2 4 SEA SSS SAM L1

=> s 12 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SCREEN SEARCH COMPLETED - 23460 TO ITERATE

100.0% PROCESSED 23460 ITERATIONS

119 ANSWERS

SEARCH TIME: 00.00.04

L3 119 SEA SSS FUL L1

=> file ca

COST IN U.S. DOLLARS '

SINCE FILE TOTAL ENTRY SESSION 133.56 133.71

FULL ESTIMATED COST

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FILE COVERS 1967 - 8 Mar 2001 VOL 134 ISS 12 FILE LAST UPDATED: 8 Mar 2001 (20010308/ED)

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=> s 13

6 L3 L4

=> s 14 and ohkawa, s?/au

235 OHKAWA, S?/AU 1 L4 AND OHKAWA, S?/AU L5

=> d 15, ibib abs hitstr, 1

ANSWER 1 OF 1 CA COPYRIGHT 2001 ACS

130:38285 CA ACCESSION NUMBER:

Benzofuran derivatives useful for suppressing TITLE:

neurodegeneration.

Ohkawa, Shigenori; Setoh, Masaki; Kakihana, INVENTOR(S):

Mitsuru; Okura, Masahiro

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 132 pp.

CODEN: PIXXD2 Patent

DOCUMENT TYPE: English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.				KIND		DATE		APPLICATION NO.				٥.	DATE				
	9855 9855					1998 1999			W	0 19	98-J	P248:	2	19980	0604		,
WO								BG,	BR,	BY,	CA,	CN,	CU,	CZ,	EE,	GE,	GW,
														MD,			
														TR,	TT,	UA,	US,
	DIAI.					AZ,								CY,	DE	DK	ES
	Lw.													BJ,			
		CM,	GA,	GN,	ML,	MR,	ΝE,	ŞN,	TD,	TG							
	AU 9875503						AU 1998-75503				19980604						
								JP 1998-155709									
EP	9882	89		A	2	2000	0329		Ε	P 19	98-9	2312	8	1998	0604		
	R:			CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,							_				_				
PRIORITY APPLN. INFO.: JP 1997-148325 19970605 WO 1998-JP2482 19980604																	
										0 19	98-J	P248	2	1998	0604		
OTHER SOURCE(S): MARPAT 130:38285																	

GΙ



$$\begin{array}{c} \text{MeO} \\ \text{Me} \\ \text{Ne} \\ \text{Ne} \\ \text{Ne} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{II} \\ \text{II}$$

AB Title compds. I [R1, R2 = H, (un)substituted hydrocarbon group; or R1 and R2 form a 3- to 8-membered carbo- or heterocyclic ring which may be substituted; R3 = H, (un)substituted lower alkyl or arom. group; R4 = (un)substituted arom. or araliph. group, or acyl; X , Y = O or S which

may

be oxidized; benzene ring may be further substituted] and their salts are disclosed. The compds. suppress .beta.-amyloid toxicity, and are thus useful as agents for treating of preventing neurodegenerative diseases such as Alzheimer's disease or Parkinsonism. Prepns. of 33 compds. I and their intermediates are described. For instance, etherification of 3-(4-isopropylphenyl)-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran-5-ol with 4-methoxybenzyl chloride using NaH in DMF gave 49% title compd. II. Seven example compds. gave 27.3-47.0% in vitro protection of human neuroblastoma SK-N-SH cells from .beta.-amyloid neurotoxicity.

IT 216989-52-5P, 3-(4-Isopropylphenyl)-2,2-dimethyl-2,3-dihydrobenzofuran-5-ol 216989-53-6P, 2,2,4,6,7-Pentamethyl-3-[4-(4-morpholinyl)phenyl]-2,3-dihydrobenzofuran-5-ol 216989-54-7P, 2,2,4,6,7-Pentamethyl-3-[4-(4-methyl-1-piperazinyl)phenyl]-2,3-dihydrobenzofuran-5-ol 216989-63-8P, 3-(4-Isopropylphenyl)-2,2-dimethyl-2,3-dihydrobenzofuran-6-ol 216989-72-9P, 5-(2,4-Diaminophenoxy)-3-(4-isopropylphenyl)-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (intermediate; prepn. of benzofuran derivs. as agents for suppressing neurodegeneration)

RN 216989-52-5 CA

CN 5-Benzofuranol, 2,3-dihydro-2,2-dimethyl-3-[4-(1-methylethyl)phenyl]-(9CI) (CA INDEX NAME)

RN 216989-53-6 CA

CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(4-

morpholinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 216989-54-7 CA

CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(4-methyl-1-piperazinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 216989-63-8 CA

CN 6-Benzofuranol, 2,3-dihydro-2,2-dimethyl-3-[4-(1-methylethyl)phenyl]-(9CI) (CA INDEX NAME)

RN 216989-72-9 CA

CN 1,3-Benzenediamine, 4-[[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-benzofuranyl]oxy]- (9CI) (CA INDEX NAME)

IT 216989-23-0P, 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-5-[[4-(methylthio)benzyl]oxy]-2,3-dihydrobenzofuran 216989-24-1P, 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-5-[[4-(methylsulfinyl)benzyl]oxy]-2,3-dihydrobenzofuran 216989-26-3P, 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-5-[(3-phenyl-2-propen-1-yl)oxy]-2,3-dihydrobenzofuran 216989-30-9P, Methyl .alpha.-[[3-(4-isopropylphenyl)-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran-5-yl]oxy]phenylacetate 216989-34-3P,

3-(4-Isopropylphenyl)-5-[(2,4-dinitrophenyl)oxy]-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran

RL: BAC (Biological activity or effector, except adverse); RCT

(Reactant);

SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(product; prepn. of benzofuran derivs. as agents for suppressing neurodegeneration)

RN 216989-23-0 CA

CN Benzofuran,

2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-[[4-(methylthio)phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 216989-24-1 CA

CN Benzofuran,

2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-[[4-(methylsulfinyl)phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 216989-26-3 CA

CN Benzofuran,
2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]5-[(3-phenyl-2-propenyl)oxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{Ph-CH} = \text{CH-CH}_2 - \text{O} \\ \text{Me} \\ \text{Me} \end{array} \qquad \begin{array}{c} \text{Pr-i} \\ \text{Me} \\$$

RN 216989-30-9 CA

CN Benzeneacetic acid, .alpha.-[[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-benzofuranyl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 216989-34-3 CA

CN Benzofuran,

5-(2,4-dinitrophenoxy)-2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

IT 216989-15-0P, 5-(Benzyloxy)-3-(4-isopropylphenyl)-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran 216989-16-1P, 5-(Benzyloxy)-3-[4-(dimethylamino)phenyl]-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran 216989-18-3P, 3-(4-Isopropylphenyl)-5-[(4-methoxybenzyl)oxy]-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran 216989-19-4P, 3-(4-Isopropylphenyl)-5-[(4-methoxybenzyl)oxy]-2,2-dimethyl-2,3-dihydrobenzofuran 216989-20-7P,

3-[4-(Dimethylamino)phenyl]-5-[(4-methoxybenzyl)oxy]-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran 216989-21-8P, 5-[(4-Methoxybenzyl)oxy]-3-[4-(4-morpholinyl)phenyl]-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran 216989-22-9P, 5-[(4-Methoxybenzyl)oxy]-2,2,4,6,7-pentamethyl-3-[4-(4-methyl-1-piperazinyl)phenyl]-2,3-dihydrobenzofuran 216989-25-2P , 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-5-[[4-(methylsulfonyl)benzyl]oxy]-2,3-dihydrobenzofuran 216989-27-4P, 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-5-(2-quinolylmethoxy)-2,3dihydrobenzofuran hydrochloride 216989-28-5P, 5-[(3,3-Diphenylpropyl)oxy]-3-(4-isopropylphenyl)-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran 216989-29-6P, Methyl 4-[[[3-(4isopropylphenyl)-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran-5yl]oxy]methyl]benzoate 216989-31-0P, 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-5-[(2-pyridylmethyl)oxy]-2,3-dihydrobenzofuran **216989-32-1P**, 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-5-[(3pyridylmethyl)oxy]-2,3-dihydrobenzofuran 216989-33-2P, 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-5-[(4-pyridylmethyl)oxy]-2,3dihydrobenzofuran 216989-35-4P, 5-[[2,4-Bis(acetylamino)phenyl]oxy]-3-(4-isopropylphenyl)-2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran 216989-36-5P 216989-37-6P **216989-38-7P**, 3-(4-1sopropylphenyl)-2, 2, 4, 6, 7-pentamethyl-5-[(3-1)]phenylpropyl)oxy]-2,3-dihydrobenzofuran 216989-39-8P, 3-(4-1) sopropylphenyl)-2,2,4,6,7-pentamethyl-5-[(2-phenylethyl)0xy]-2,3dihydrobenzofuran 216989-43-4P, 3-(4-Isopropylphenyl)-6-{(4methoxybenzyl)oxy]-2,2-dimethyl-2,3-dihydrobenzofuran RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (product; prepn. of benzofuran derivs. as agents for suppressing neurodegeneration) RN 216989-15-0 CA Benzofuran, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-

5-(phenylmethoxy)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{Me} \\ & \text{Me} & \text{Pr-i} \\ & \text{Ph-CH}_2-0 & \text{Me} \end{array}$$

RN 216989-16-1 CA

CN Benzenamine, 4-[2,3-dihydro-2,2,4,6,7-pentamethyl-5-(phenylmethoxy)-3-benzofuranyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

RN 216989-18-3 CA

CN Benzofuran,

2,3-dihydro-5-[(4-methoxyphenyl)methoxy]-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 216989-19-4 CA

CN Benzofuran,

2,3-dihydro-5-[(4-methoxyphenyl)methoxy]-2,2-dimethyl-3-[4-(1methylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 216989-20-7 CA

CN Benzenamine, 4-[2,3-dihydro-5-[(4-methoxyphenyl)methoxy]-2,2,4,6,7-pentamethyl-3-benzofuranyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

RN 216989-21-8 CA

CN Morpholine, 4-[4-[2,3-dihydro-5-[(4-methoxyphenyl)methoxy]-2,2,4,6,7-pentamethyl-3-benzofuranyl]phenyl]- (9CI) (CA INDEX NAME)

RN 216989-22-9 CA

CN Piperazine, 1-[4-[2,3-dihydro-5-[(4-methoxyphenyl)methoxy]-2,2,4,6,7-pentamethyl-3-benzofuranyl]phenyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 216989-25-2 CA

CN Benzofuran,

2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]- 5-[[4-(methylsulfonyl)phenyl]methoxy]- (9CI) (CA INDEX NAME)

RN 216989-27-4 CA

CN Quinoline, 2-[[[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-benzofuranyl]oxy]methyl]-, hydrochloride (9CI) (CAINDEX NAME)

HC1

RN 216989-28-5 CA

CN Benzofuran,

5-(3,3-diphenylpropoxy)-2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{Me} \\ \text{Me} & \text{O} & \text{Me} \\ \text{Ph}_2\text{CH}-\text{CH}_2-\text{CH}_2-\text{O} & \text{Me} \\ \text{Me} & \text{Me} \end{array}$$

RN 216989-29-6 CA

CN Benzoic acid, 4-[[[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1methylethyl)phenyl]-5-benzofuranyl]oxy]methyl]-, methyl ester (9CI) (CA
INDEX NAME)

RN 216989-31-0 CA

CN Pyridine, 2-[[[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-benzofuranyl}oxy]methyl]- (9CI) (CA INDEX NAME)

RN 216989-32-1 CA

CN Pyridine, 3-[[[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-benzofuranyl]oxy]methyl]- (9CI) (CA INDEX NAME)

RN 216989-33-2 CA

CN Pyridine, 4-[[[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-benzofuranyl]oxy]methyl]- (9CI) (CA INDEX NAME)

RN 216989-35-4 CA
CN Acetamide, N,N'-[4-[[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methyl-thyl)phenyl]-5-benzofuranyl]oxy]-1,3-phenylene]bis- (9CI) (CA INDEX NAME)

RN 216989-36-5 CA
CN Benzeneacetic acid,
.alpha.-[[(3R)-2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-benzofuranyl]oxy]-, (.alpha.R)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 216989-37-6 CA
CN Benzeneacetic acid,
.alpha.-[[(3R)-2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4(1-methylethyl)phenyl]-5-benzofuranyl]oxy]-, (.alpha.S)-rel- (9CI) (CA
INDEX NAME)

Relative stereochemistry.

RN 216989-38-7 CA

CN Benzofuran,

2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-(3-phenylpropoxy)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{O} \\ \text{Me} \\ \text{Ph- (CH}_2)_3 - \text{O} \\ \text{Me} \\ \end{array}$$

RN 216989-39-8 CA

CN Benzofuran,

2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]-5-(2-phenylethoxy)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{Ph-CH}_2-\text{CH}_2-\text{O} \\ \text{Me} \\ \end{array}$$

RN 216989-43-4 CA

CN Benzofuran,

2,3-dihydro-6-[(4-methoxyphenyl)methoxy]-2,2-dimethyl-3-[4-(1methylethyl)phenyl]- (9CI) (CA INDEX NAME)

IT 116674-35-2, 3-(4-Isopropylphenyl)-2,2,4,6,7-pentamethyl-2,3dihydrobenzofuran-5-ol 116674-53-4, 3-[4-(Dimethylamino)phenyl]2,2,4,6,7-pentamethyl-2,3-dihydrobenzofuran-5-ol
RL: RCT (Reactant)

(starting material; prepn. of benzofuran derivs. as agents for suppressing neurodegeneration) $\,$

RN 116674-35-2 CA

CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1methylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 116674-53-4 CA

CN 5-Benzofuranol, 3-[4-(dimethylamino)phenyl]-2,3-dihydro-2,2,4,6,7pentamethyl- (9CI) (CA INDEX NAME)

=> d his

(FILE 'HOME' ENTERED AT 17:20:08 ON 14 MAR 2001)

FILE 'REGISTRY' ENTERED AT 17:20:11 ON 14 MAR 2001

- L1 STRUCTURE UPLOADED
- L2 4 S L1
- L3 119 S L2 FULL

FILE 'CA' ENTERED AT 17:20:57 ON 14 MAR 2001

6 S L3

L5 1 S L4 AND OHKAWA, S?/AU

=> s 14 not 15

L6 5 L4 NOT L5

=> d 16, ibib abs hitstr, 1-5

L6 ANSWER 1 OF 5 CA COPYRIGHT 2001 ACS

ACCESSION NUMBER: 109:149335 CA
TITLE: Preparation of 5-hydroxycoumaran derivatives as cardiovascular and antiallergy agents

INVENTOR(S):

Terao, Shinji; Maki, Yoshitaka PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

Eur. Pat. Appl., 39 pp.

SOURCE:

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
	A1	19880706	EP 1987-311122	19871217	
	B1	19920311	en in it iii Ni	C.E.	
The state of the s			R, IT, LI, LU, NL JP 1987-310346		
JP 01272578	A2	19891031	JP 1987-310346	190/120/	
JP 08005871	B4	19960124			
AT 73448	E	19920315	AT 1987-311122	19871217	
DK 8706789	Α	19880628	DK 1987-6789	19871222	
US 4857516	Α	19890815	US 1987-136273	19871222	
ни 48609	A2	19890628	HU 1987-5988	19871223	
HU 206332	В	19921028			
AU 8783040	Ā1	19880630	AU 1987-83040	19871224	
AU 605818	B2	19910124			
CA 1325635	A1	19931228	CA 1987-555354	19871224	
PRIORITY APPLN. INFO			JP 1986-313380	19861227	
			JP 1987-235491	19870918	
			EP 1987-311122	19871217	
OTHER SOURCE(S):	MA	RPAT 109:149335			

$$R^{00}$$
 R^{00}
 R

AB The title compds. [I; R = alkyl; R0 = H, acyl; R1-R4 = (un)substituted alkyl; R1R2 = CH:CHCH:CH; R3R4 = polymethylene; R5 = (un)substituted alkyl, aryl, heterocyclyl] were prepd. 4-FC6H4COCHMe2 (prepn. given) was added to 1-bromo-2,5-dimethoxy-3,4,6-trimethylbenzene in THF previously treated with BuLi and the mixt. stirred 1 h to give 92.3%

diphenylpropanol
II which was refluxed 18 h in 47 wt.% aq. HBr to give 74.8% title compd.
III. The latter, at 100 mg/kg orally gave 93% inhibition of the
excitatory behavior induced by spinal intrathecal injection of FeC12

soln.

IT 116674-24-9P 116707-50-7P 116707-51-8P 116707-52-9P 116707-53-0P 116707-54-1P 116707-55-2P 116707-56-3P 116707-57-4P 116707-58-5P 116707-59-6P 116707-60-9P 116707-61-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction of, in prepn. of cardiovascular and antiallergic agents)

RN 116674-24-9 CA

CN 5-Benzofuranol, 3-(4-fluorophenyl)-2,3-dihydro-2,4,6,7-tetramethyl-2-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 116707-50-7 CA

CN Benzofuran, 3-(4-bromophenyl)-2,3-dihydro-5-(methoxymethoxy)-2,2,4,6,7-pentamethyl- (9CI) (CA INDEX NAME)

RN 116707-51-8 CA

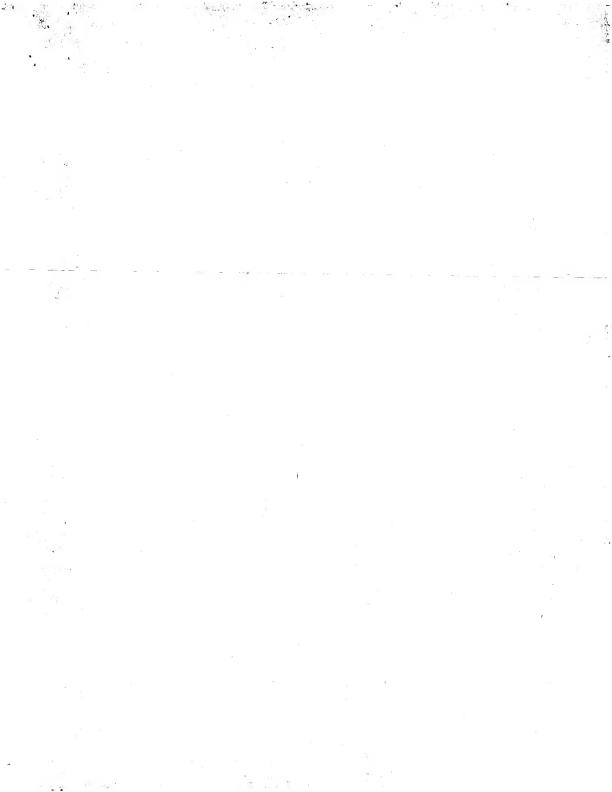
CN Benzaldehyde, 4-(2,3-dihydro-5-methoxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

RN 116707-52-9 CA

CN Benzenemethanol, 4-(2,3-dihydro-5-methoxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

RN 116707-53-0 CA

CN Benzofuran, 3-[4-(bromomethyl)phenyl]-2,3-dihydro-5-methoxy-2,2,4,6,7pentamethyl- (9CI) (CA INDEX NAME)



116707-54-1 CA RN

Benzeneacetonitrile, 4-(2,3-dihydro-5-methoxy-2,2,4,6,7-pentamethyl-3-CN benzofuranyl) - (9CI) (CA INDEX NAME)

RN

116707-55-2 CA Benzofuran, 2,3-dihydro-5-methoxy-2,2,4,6,7-pentamethyl-3-[4-CN [(phenylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 116707-56-3 CA

2-Cyclohexene-1-carboxylic acid, 2-[4-(2,3-dihydro-5-methoxy-2,2,4,6,7-CN pentamethy1-3-benzofuranyl)phenyl]- (9CI) (CA INDEX NAME)

RN 116707-57-4 CA

CN Piperidine, 1-[[4-(2,3-dihydro-5-methoxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 116707-58-5 CA

CN 2-Propenoic acid, 3-[4-(2,3-dihydro-5-methoxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 116707-59-6 CA

CN Benzeneheptanoic acid, 4-(2,3-dihydro-5-methoxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

RN 116707-60-9 CA

CN Benzenepropanoic acid, 4-(2,3-dihydro-5-methoxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 116707-61-0 CA
CN Benzoic acid, 4-[2,3-dihydro-5-(methoxymethoxy)-2,2,4,6,7-pentamethyl-3benzofuranyl]- (9CI) (CA INDEX NAME)

116674-16-9P 116674-19-2P 116674-21-6P IT 116674-22-7P 116674-23-8P 116674-26-1P 116674-28-3P 116674-29-4P 116674-30-7P 116674-31-8P 116674-32-9P 116674-33-0P 116674-34-1P 116674-35-2P 116674-36-3P 116674-37-4P 116674-38-5P 116674-39-6P 116674-40-9P 116674-41-0P 116674-42-1P 116674-43-2P 116674-44-3P 116674-45-4P 116674-46-5P 116674-47-6P 116674-48-7P 116674-49-8P 116674-50-1P 116674-51-2P 116674-52-3P 116674-53-4P 116674-54-5P 116674-55-6P 116674-56-7P 116674-57-8P 116674-58-9P 116674-59-0P 116674-60-3P 116674-61-4P 116674-62-5P 116674-63-6P 116674-64-7P 116674-65-8P 116674-66-9P 116706-84-4P 116706-85-5P 116706-86-6P 116706-87-7P 116706-88-8P 116706-89-9P 116706-90-2P 116706-91-3P 116728-40-6P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as cardiovascular and antiallergic agent) 116674-16-9 CA RN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(3-pyridinyl)- (9CI) CN (CA INDEX NAME)

RN 116674-19-2 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 116674-21-6 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-phenyl- (9CI) (CA INDEX NAME)

RN 116674-22-7 CA CN 5-Benzofuranol, 3-(4-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

RN 116674-23-8 CA

CN 5-Benzofuranol, 3-(4-fluorophenyl)-2,3-dihydro-2,4,6,7-tetramethyl-2-pentyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 116674-26-1 CA

CN 5-Benzofuranol, 3-(4-bromophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI)

(CA INDEX NAME)

RN 116674-28-3 CA

CN 5-Benzofuranol, 3-(4-chlorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

RN 116674-29-4 CA

CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 116674-30-7 CA CN 5-Benzofuranol, 3-(2-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

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RN 116674-31-8 CA CN 5-Benzofuranol, 3-(3-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

RN 116674-32-9 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(4-methylphenyl)-(9CI) (CA INDEX NAME)

RN 116674-33-0 CA

CN 5-Benzofuranol, 3-(4-ethylphenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

RN 116674-34-1 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(4-propylphenyl)-(9CI) (CA INDEX NAME)

RN 116674-35-2 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 116674-36-3 CA CN 5-Benzofuranol, 3-[4-(1,1-dimethylethyl)phenyl]-2,3-dihydro-2,2,4,6,7-pentamethyl- (9CI) (CA INDEX NAME)

RN 116674-37-4 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(4-pentylphenyl)-(9CI) (CA INDEX NAME)

Me Me Me HO Me (CH₂)
$$_4$$
 - Me

RN 116674-38-5 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(4-octylphenyl)-(9CI) (CA INDEX NAME)

Me Me Me
$$(CH_2)_7$$
 - Me

RN 116674-39-6 CA CN 5-Benzofuranol, 3-(4-decylphenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

Me Me Me
$$(CH_2)_9$$
 - Me

RN 116674-40-9 CA CN 5-Benzofuranol, 3-(4-dodecylphenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

RN 116674-41-0 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(4-tetradecylphenyl)-(9CI) (CA INDEX NAME)

RN 116674-42-1 CA CN 5-Benzofuranol, 3-(4-hexadecylphenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

Me Me Me
$$(CH_2)_{15}$$
 Me $(CH_2)_{15}$ Me

RN 116674-43-2 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(4-octadecylphenyl)-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{HO} \\ \text{Me} \\ \text{(CH2)} \\ 17-\text{Me} \end{array}$$

RN 116674-44-3 CA CN 5-Benzofuranol, 2,3-dihydro-3-(4-hydroxyphenyl)-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

RN 116674-45-4 CA
CN 5-Benzofuranol, 2,3-dihydro-3-(3-hydroxyphenyl)-2,2,4,6,7-pentamethyl(9CI) (CA INDEX NAME)

RN 116674-46-5 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(methylthio)phenyl]-(9CI) (CA INDEX NAME)

RN 116674-47-6 CA CN 5-Benzofuranol, 3-(3,4-dimethylphenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

RN 116674-48-7 CA CN 5-Benzofuranol, 3-(2,3-dihydro-1H-inden-5-yl)-2,3-dihydro-2,2,4,6,7-pentamethyl- (9CI) (CA INDEX NAME)

RN 116674-49-8 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(5,6,7,8-tetrahydro-2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 116674-50-1 CA CN 5-Benzofuranol, 3-cyclohexyl-2,3-dihydro-2,2,4,6,7-pentamethyl- (9CI) (CA INDEX NAME)

RN 116674-51-2 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(1-naphthalenyl)-(9CI) (CA INDEX NAME)

RN 116674-52-3 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(2-naphthalenyl)-(9CI) (CA INDEX NAME)

RN 116674-53-4 CA CN 5-Benzofuranol, 3-[4-(dimethylamino)phenyl]-2,3-dihydro-2,2,4,6,7-pentamethyl- (9CI) (CA INDEX NAME)

RN 116674-54-5 CA CN 5-Benzofuranol, 3-(4-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-, acetate (9CI) (CA INDEX NAME)

RN 116674-55-6 CA CN Propanoic acid, 2-methyl-, 3-(4-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-5-benzofuranyl ester (9CI) (CA INDEX NAME)

RN 116674-56-7 CA CN Cyclohexanecarboxylic acid, 3-(4-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-5-benzofuranyl ester (9CI) (CA INDEX NAME)

RN 116674-57-8 CA
CN Decanoic acid, 3-(4-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-5-benzofuranyl ester (9CI) (CA INDEX NAME)

RN 116674-58-9 CA CN 5-Benzofuranol, 3-(4-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-, benzoate (9CI) (CA INDEX NAME)

RN 116674-59-0 CA CN 3-Pyridinecarboxylic acid, 3-(4-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-5-benzofuranyl ester (9CI) (CA INDEX NAME)

RN 116674-60-3 CA
CN Pyridinium,
3-(2,3-dihydro-5-hydroxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)1-methyl-, iodide (9CI) (CA INDEX NAME)

• I-

RN 116674-61-4 CA
CN Benzaldehyde, 4-(2,3-dihydro-5-hydroxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

RN 116674-62-5 CA
CN Benzoic acid, 4-(2,3-dihydro-5-hydroxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

RN 116674-63-6 CA
CN Benzeneacetic acid, 4-(2,3-dihydro-5-hydroxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

RN 116674-64-7 CA

CN 2-Propenoic acid, 3-[4-(2,3-dihydro-5-hydroxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO} \\ \text{Me} \\ \text{HO} \\ \text{Me} \\ \text{CH---} \text{CH---} \text{CO}_2\text{H} \\ \end{array}$$

RN 116674-65-8 CA

CN Benzenepropanoic acid, 4-(2,3-dihydro-5-hydroxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{HO} \\ \text{Me} \\ \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \end{array}$$

RN 116674-66-9 CA

CN Benzeneheptanoic acid, 4-(2,3-dihydro-5-hydroxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

RN 116706-84-4 CA

CN 5-Benzofuranol, 3-(2,4-dimethylphenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-(9CI) (CA INDEX NAME)

RN 116706-85-5 CA

CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-piperidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 116706-86-6 CA

5-Benzofuranol, 2,3-dihydro-3-[4-(hydroxymethyl)phenyl]-2,2,4,6,7-pentamethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{HO} \\ \text{Me} \\ \text{CH}_2-\text{OH} \end{array}$$

RN 116706-87-7 CA

CN 2-Propenoic acid, 3-[4-(2,3-dihydro-5-hydroxy-2,2,4,6,7-pentamethyl-3-benzofuranyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

116706-88-8 CA RN

Butanedioic acid, mono[2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-(1-CN methylethyl)phenyl]-5-benzofuranyl] ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{Me} \\ & \text{Me} & \text{O} & \text{Me} \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2-\text{C}-\text{O} & \text{Me} \\ & \text{Me} & \text{Pr-i} \end{array}$$

116706-89-9 CA RN

5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-(3-pyridinyl)-, CN hydrochloride (9CI) (CA INDEX NAME)

HC1

RN 116706-90-2 CA

5-Benzofuranol, 3-[4-(dimethylamino)phenyl]-2, 3-dihydro-2, 2, 4, 6, 7-dihydro-2, 4, 7-dihydro-2CN pentamethyl-, hydrochloride (9CI) (CA INDEX NAME)

• HCl

RN 116706-91-3 CA .
CN Pyridinium, 3-[[[3-(4-fluorophenyl)-2,3-dihydro-2,2,4,6,7-pentamethyl-5-benzofuranyl]oxy]carbonyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)

• I-

RN 116728-40-6 CA CN 5-Benzofuranol, 2,3-dihydro-2,2,4,6,7-pentamethyl-3-[4-[(phenylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)

L6 ANSWER 2 OF 5 CA COPYRIGHT 2001 ACS ACCESSION NUMBER: 108:112209 CA

TITLE:

2,3-dihydrobenzofuran

obenzofuran
derivatives from resorcinol derivatives

A process for the preparation of

INVENTOR(S): Takahashi, Katsuya; Hashimoto, Isao

PATENT ASSIGNEE(S): Mitsui Petrochemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62138487	A2	19870622	JP 1985-279193	19851213
JP 04046273	B4	19920729		

GI For diagram(s), see printed CA Issue.

AB The title compds. (I), useful as intermediates for agrochems.,

pharmaceuticals, and perfumes, are prepd. from 1,3-dihydroxybenzenes (II).

113168-21-1P 113168-22-2P 113168-23-3P 113168-24-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by cyclocondensation of resorcinol with ketone)

RN 113168-21-1 CA

CN 6-Benzofuranol, 2,3-dihydro-2,2-dimethyl-3-phenyl- (9CI) (CA INDEX NAME)

RN 113168-22-2 CA

CN 6-Benzofuranol, 3-(2-chlorophenyl)-2,3-dihydro-2,2-dimethyl- (9CI) (CA INDEX NAME)

RN 113168-23-3 CA

CN 6-Benzofuranol, 2,3-dihydro-2,2-dimethyl-3-(2-methylphenyl)- (9CI) (CA INDEX NAME)

113168-24-4 CA 6-Benzofuranol, 2,3-dihydro-3-(4-methoxyphenyl)-2,2-dimethyl- (9CI) (CA CN INDEX NAME)

ANSWER 3 OF 5 CA COPYRIGHT 2001 ACS

ACCESSION NUMBER:

105:226586 CA

TITLE:

Bicyclic benzoxy heterocyclic ethers and thioethers

H2-receptor antagonists

INVENTOR(S):

Kuhla, Donald Ernest; Campbell, Henry Flud; Studt,

William Lyon; Neuenschwander, Kent William Rorer International (Overseas), Inc., USA

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8602550	A1	19860509	WO 1985-US2080	19851022
W: AU, JP RW: AT, BE,	CH, DE	, FR, GB, IT,	LU, NL, SE	
US 4612309	A	19860916	US 1984-664063	19841023
AU 8550688	A1	19860515	AU 1985-50688	19851022
AU 578199	B2	19881013		
EP 198918	A1	19861029	EP 1985-905731	19851022
R: AT, BE,	CH, DE	, FR, GB, IT,	LI, LU, NL, SE	
JP 62500593	T2	19870312	JP 1985-505036	19851022
US 4668673	Α	19870526	US 1986-881122	19860702
US 4722925	A	19880202	US 1987-21147	19870303
US 4777168	A	19881011	US 1988-142084	19880107
PRIORITY APPLN. INFO	.:		US 1984-664063	19841023
			WO 1985-US2080	19851022
			US 1986-881122	19860702

GΙ

AB Title compds. I [R, R1 = H, alkyl; R2 = NHR4, amino, N-contg. heterocycle,

amidino; R3 = amino, amidino; R4 = amidino, thiocarboxamidino, cyclobutendionyl, N- or N,S-contg. heterocycle; n=1,2; p=0,1; q=2-4; m=0-2; X=0, S, S(0), S(0)2], useful as H2-receptor antagonists (no data), are prepd. Thus, 6-methoxy-4-benzopyranone was hydrogenated

give benzopyran II (R5 = OMe, R6 = OH), which was mesylated and treated with piperidine to give II (R5 = OMe, R6 = piperidino). This was demethylated and alkylated to yield II (R5 = OCH2CH2CH2Br, R6 = piperidino), which was treated with NaN3 and reduced to form II (R5 = OCH2CH2CH2NH2, R6 = piperidino). This was cyclized with PhCH:NNMeC(:NCN)SMe to give benzopyranyloxypropylaminotriazole III.

RN 105329-74-6 CA

CN 7-Benzofuranol, 2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)- (9CI) (CA INDEX NAME)

IT 105329-85-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and cyclization of)

RN 105329-85-9 CA

ON Acetamide, 2-(acetyloxy)-N-[[[4-[[2,3-dihydro-2,2-dimethyl-3-(1-

piperidinyl)-7-benzofuranyl]oxy]butyl]amino][methyl(phenylmethylene)hydraz ino]methylene]- (9CI) (CA INDEX NAME)

IT 105329-80-4P 105350-84-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and cyclocondensation of, with carboximidothioic acid deriv.)

RN 105329-80-4 CA

CN 1-Butanamine, 4-[[2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)-7-benzofuranyl]oxy]- (9CI) (CA INDEX NAME)

RN 105350-84-3 CA

CN 1-Propanamine, 3-[[2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)-7-benzofuranyl]oxy]- (9CI) (CA INDEX NAME)

IT 105329-73-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and demethylation of)

RN 105329-73-5 CA

CN Piperidine, 1-(2,3-dihydro-7-methoxy-2,2-dimethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

• HCl

IT 105329-76-8P 105329-79-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and hydride redn. of)

RN 105329-76-8 CA

CN Piperidine,

1-[7-(3-azidopropoxy)-2,3-dihydro-2,2-dimethyl-3-benzofuranyl]-(9CI) (CA INDEX NAME)

RN 105329-79-1 CA

CN Piperidine,

IT 105329-75-7P 105329-78-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction of, with azide)

RN 105329-75-7 CA

CN Piperidine,

1-[7-(3-bromopropoxy)-2,3-dihydro-2,2-dimethyl-3-benzofuranyl]-(9CI) (CA INDEX NAME)

RN 105329-78-0 CA

CN Piperidine,

1-[7-(4-bromobutoxy)-2,3-dihydro-2,2-dimethyl-3-benzofuranyl](9CI) (CA INDEX NAME)

IT 105329-70-2P 105329-77-9P 105329-81-5P 105329-82-6P 105329-83-7P 105329-84-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as H2 receptor antagonist for ulcer treatment)

RN 105329-70-2 CA

CN 1H-1,2,4-Triazole-3,5-diamine, N5-[3-[[2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)-7-benzofuranyl]oxy]propyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 105329-77-9 CA

CN 3-Cyclobutene-1,2-dione, 3-amino-4-[[3-[[2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)-7-benzofuranyl]oxy]propyl]amino]- (9CI) (CA INDEX NAME)

RN 105329-81-5 CA CN 1H-1,2,4-Triazole-3,5-diamine, N5-[4-[[2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)-7-benzofuranyl]oxy]butyl]-1-methyl- (9CI) (CA INDEX NAME)

RN 105329-82-6 CA CN 3-Cyclobutene-1,2-dione, 3-amino-4-[[4-[[2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)-7-benzofuranyl]oxy]butyl]amino]- (9CI) (CA INDEX NAME)

RN 105329-83-7 CA CN 1,2,5-Thiadiazole-3,4-diamine, N-[4-[[2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)-7-benzofuranyl]oxy]butyl]-, 1-oxide (9CI) (CA INDEX NAME)

RN 105329-84-8 CA
CN 1H-1,2,4-Triazole-3-methanol, 5-[[4-[[2,3-dihydro-2,2-dimethyl-3-(1-piperidinyl)-7-benzofuranyl]oxy]butyl]amino]-1-methyl- (9CI) (CA INDEX NAME)

L6 ANSWER 4 OF 5 CA COPYRIGHT 2001 ACS

ACCESSION NUMBER:

81:135855 CA

TITLE:

Benzoheterocyclic derivatives. 15. Synthesis of

benzofuran derivatives. 3

AUTHOR(S):

Hirose, Noriyasu; Kuriyama, Shizuo; Sohda, Shigeru Res. Lab., Eisai Co., Ltd., Tokyo, Japan

CORPORATE SOURCE: Res. Lab., Eisai Co., Ltd., Tokyo, Jay SOURCE: Yakugaku Zasshi (1974), 94(8), 905-12

CODEN: YKKZAJ

DOCUMENT TYPE:

Journal

LANGUAGE:

Japanese

GI For diagram(s), see printed CA Issue.

AB 3-Substituted amino— or aminomethyl-2,3-dihydrobenzofurans I (R = OCH2CH2NMe2, substituted amino, substituted aminomethyl; R1 = H, Me) were prepd. Special emphasis was placed on the 5-position, which corresponds to the meta position of the phenethylamine skeleton. I (R = CN, R1 = Me) was obtained in a good yield by cyanation of I (R = Br, R1 = Me) with CuCN. The analgesic effect of these benzofuran derivs. was comparable to that of aminopyrine.

IT 53903-28-9P 53903-29-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 53903-28-9 CA

CN Piperidine, 1-(2,3-dihydro-5-methoxy-2,2-dimethyl-3-benzofuranyl)- (9CI) (CA INDEX NAME)

RN 53903-29-0 CA

CN Piperidine, 1-(2,3-dihydro-5-methoxy-2,2-dimethyl-3-benzofuranyl)-,
 ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

53903-28-9 CRN CMF C16 H23 N O2

CM 2

CRN 144-62-7 CMF C2 H2 O4

ANSWER 5 OF 5 CA COPYRIGHT 2001 ACS

ACCESSION NUMBER:

75:63523 CA

AUTHOR(S):

Photolysis of

2-(benzyloxy)-4-(dodecyloxy)benzophenone

and 2-isopropoxy-4-methoxybenzophenone

Lappin, Gerald R.; Zannucci, J. S.

CORPORATE SOURCE:

Tennessee Eastman Co. Div., Eastman Kodak Co.,

Kingsport, Tenn., USA

SOURCE:

J. Org. Chem. (1971), 36(13), 1808-11

CODEN: JOCEAH

DOCUMENT TYPE:

Journal

LANGUAGE:

English

For diagram(s), see printed CA Issue. GΙ

The photolysis of 2-(benzyloxy)-4-(dodecyloxy)benzophenone (I) or of AB 2-isopropoxy-4-methoxybenzophenone (II) proceeded mainly via ring closure between the carbonyl C and the .alpha. carbon of the 2 substituent to

give

6-(dodecyloxy)-2,3-dihydro-2,3-diphenyl-3-benzofuranol (III) or 2,3-dihydro-2,2-dimethyl-6-methoxy-3-phenyl-3-benzofuranol (IV), resp. The quantum efficiencies for disappearance of starting ketone and for cyclization decreased significantly with an increase in solvent polarity. The lifetime of the excited state, believed to be 3(n, .pi.*), was about

3

.times. 10-8 sec, unusually short for a benzophenone. Further photolysis of I or III resulted in dehydration to give 6-(dodecyloxy)-2,3diphenylbenzofuran (V) and partial cyclization of V to 11-(dodecyloxy)benzo[b]phenanthro[9,10-d] furan, but further photolysis

of

IV gave only 2-hydroxy-4-methoxybenzophenone. Both I and II gave the corresponding 4-alkoxy-2-hydroxybenzophenone as a minor product.

IT 28856-53-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 28856-53-3 CA

CN 3-Benzofuranol, 2,3-dihydro-6-methoxy-2,2-dimethyl-3-phenyl- (8CI) (CA INDEX NAME)

=> file reg

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
26.66 160.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL

ENTRY SESSION
CA SUBSCRIBER PRICE -3.36 -3.36

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TSCA INFORMATION NOW CURRENT THROUGH July 8, 2000

Please note that search-term pricing does apply when conducting ${\tt SmartSELECT}$ searches.

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Uploading 9445193a.str

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS L7 STR

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G2 Cy
```

G1 O,S G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 17:24:04 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 7607 TO ITERATE

13.1% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 146921 TO 157359 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 18 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 133.25 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 17:24:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 152467 TO ITERATE

100.0% PROCESSED 152467 ITERATIONS

135 ANSWERS

SEARCH TIME: 00.00.12

L9 135 SEA SSS FUL L7

=> d his

(FILE 'HOME' ENTERED AT 17:20:08 ON 14 MAR 2001)

FILE 'REGISTRY' ENTERED AT 17:20:11 ON 14 MAR 2001

L1 STRUCTURE UPLOADED

L2 4 S L1 L3 119 S L2 FULL FILE 'CA' ENTERED AT 17:20:57 ON 14 MAR 2001

L4 6 S L3

L5 1 S L4 AND OHKAWA, S?/AU

L6 5 S L4 NOT L5

FILE 'REGISTRY' ENTERED AT 17:23:30 ON 14 MAR 2001

L7 STRUCTURE UPLOADED

L8 0 S L7

L9 135 S L8 FULL

=> file ca

SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION FULL ESTIMATED COST 133.87 294.24 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -3.36CA SUBSCRIBER PRICE 0.00

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8 L9 L10

=> d his

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FILE 'REGISTRY' ENTERED AT 17:20:11 ON 14 MAR 2001

STRUCTURE UPLOADED L1

4 S L1 L2

119 S L2 FULL L3

FILE 'CA' ENTERED AT 17:20:57 ON 14 MAR 2001

L46 S L3

1 S L4 AND OHKAWA, S?/AU L5

5 S L4 NOT L5 L6

FILE 'REGISTRY' ENTERED AT 17:23:30 ON 14 MAR 2001

L7 STRUCTURE UPLOADED

0 S L7 L8

L9 135 S L8 FULL

FILE 'CA' ENTERED AT 17:24:35 ON 14 MAR 2001

L10 8 S L9

=> s 110 not 14

2 L10 NOT L4 L11

=> d lll, ibib abs hitstr, 1-2

L11 ANSWER 1 OF 2 CA COPYRIGHT 2001 ACS

119:270938 CA ACCESSION NUMBER:

An expedient route to spirobenzofurans TITLE:

Sumathi, T.; Balasubramanian, K. K. AUTHOR(S):

Journal

CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Madras, 600 036,

India

Tetrahedron Lett. (1993), 34(24), 3915-8 SOURCE:

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

GI

English CASREACT 119:270938

$$R^2$$
 OH R^2 OH R^2 COR II

The synthesis of spirobenzofurans I (R = H, Me, Ph; R1 = H, C1, Me, OMe; AB R2 = H, OMe) via base-mediated spiroannulation of arom. aldehydes and ketones II with 2-chlorocyclohexanone is reported. ΙT 151424-49-6P 151424-50-9P 151424-51-0P RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

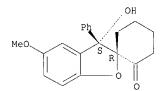
RN 151424-49-6 CA

Spiro[benzofuran-2(3H), 1'-cyclohexan]-2'-one,

3-hydroxy-5-methoxy-3-phenyl-

, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



151424-50-9 CA RN Spiro[benzofuran-2(3H),1'-cyclohexan]-2'-one, 3-hydroxy-6-methoxy-3-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 151424-51-0 CA

Spiro[benzofuran-2(3H),1'-cyclohexan]-2'-one, 3-hydroxy-5,6-dimethoxy-3phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L11 ANSWER 2 OF 2 CA COPYRIGHT 2001 ACS ACCESSION NUMBER: 117:26220 CA

ACCESSION NUMBER: 117:26220 CA
TITLE: A photochemical entry to spirobenzofurans

AUTHOR(S): Sumathi, T.; Balasubramanian, K. K.

CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Madras, 600 036,

India

SOURCE: Tetrahedron Lett. (1992), 33(16), 2213-16

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:26220

GΙ

AB Synthesis of spirobenzofurans based on photochem. .delta. hydrogen abstraction is reported. Thus, irradn. in Et2O of (cyclohexenyloxy)benzophenones I (R1 = H, OMe; R2 = H, C1, Me) gave a mixt. of diastereomeric spirobenzofuranols II.

IT 141883-82-1P 141883-83-2P 141883-84-3P

141883-85-4P
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of) N 141883-82-1 CA

CN Spiro[benzofuran-2(3H),1'-[2]cyclohexen]-3-ol, 6-methoxy-3-phenyl-, trans-

(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 141883-83-2 CA CN Spiro[benzofuran-2(3H),1'-[2]cyclohexen]-3-ol, 6-methoxy-3-phenyl-, cis-

(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 141883-84-3 CA

CN Spiro[benzofuran-2(3H),1'-[2]cyclohexen]-3-ol, 5-methoxy-3-phenyl-, trans-

(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 141883-85-4 CA

CN Spiro[benzofuran-2(3H),1'-[2]cyclohexen]-3-ol, 5-methoxy-3-phenyl-, cis-(9CI) (CA INDEX NAME)

Relative stereochemistry.

=> file ca

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	8.29	302.53
DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
DISCOUNT AMOUNTS (FOR QUALIFITING ACCOUNTS)	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.12	-4.48

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=> d his

1.7

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FILE 'REGISTRY' ENTERED AT 17:20:11 ON 14 MAR 2001 L1 STRUCTURE UPLOADED

L2 4 S L1

L3 119 S L2 FULL

FILE 'CA' ENTERED AT 17:20:57 ON 14 MAR 2001

L4 6 S L3

L5 1 S L4 AND OHKAWA, S?/AU

L6 5 S L4 NOT L5

FILE 'REGISTRY' ENTERED AT 17:23:30 ON 14 MAR 2001

STRUCTURE UPLOADED

L8 0 S L7

L9 135 S L8 FULL

FILE 'CA' ENTERED AT 17:24:35 ON 14 MAR 2001

L10 8 S L9

L11 2 S L10 NOT L4

FILE 'CA' ENTERED AT 17:25:21 ON 14 MAR 2001

=> s 19

L12 8 L9

=> file caold

COST IN U.S. DOLLARS

SINCE FILE
ENTRY
SESSION
70.31

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
SINCE FILE
ENTRY
SESSION

CA SUBSCRIBER PRICE 0.00 -4.48

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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=> d his

L1

L7

(FILE 'HOME' ENTERED AT 17:20:08 ON 14 MAR 2001)

FILE 'REGISTRY' ENTERED AT 17:20:11 ON 14 MAR 2001

STRUCTURE UPLOADED

L2 4 S L1

L3 119 S L2 FULL

FILE 'CA' ENTERED AT 17:20:57 ON 14 MAR 2001

L4 6 S L3

L5 1 S L4 AND OHKAWA, S?/AU

L6 5 S L4 NOT L5

FILE 'REGISTRY' ENTERED AT 17:23:30 ON 14 MAR 2001

STRUCTURE UPLOADED

L8 0 S L7

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135 S L8 FULL
L9
    FILE 'CA' ENTERED AT 17:24:35 ON 14 MAR 2001
             8 S L9
L10
              2 S L10 NOT L4
L11
    FILE 'CA' ENTERED AT 17:25:21 ON 14 MAR 2001
             8 S L9
L12
     FILE 'CAOLD' ENTERED AT 17:25:37 ON 14 MAR 2001
=> s 19
L13
           0 L9
=> d his
     (FILE 'HOME' ENTERED AT 17:20:08 ON 14 MAR 2001)
     FILE 'REGISTRY' ENTERED AT 17:20:11 ON 14 MAR 2001
               STRUCTURE UPLOADED
L1
             4 S L1
L2
           119 S L2 FULL
L3
     FILE 'CA' ENTERED AT 17:20:57 ON 14 MAR 2001
             6 S L3
L4
              1 S L4 AND OHKAWA, S?/AU
L5
              5 S L4 NOT L5
L6
     FILE 'REGISTRY' ENTERED AT 17:23:30 ON 14 MAR 2001
               STRUCTURE UPLOADED
L7
              0 S L7
\Gamma8
L9
           135 $ L8 FULL
     FILE 'CA' ENTERED AT 17:24:35 ON 14 MAR 2001
L10
             8 S L9
              2 S L10 NOT L4
L11
     FILE 'CA' ENTERED AT 17:25:21 ON 14 MAR 2001
             8 S L9
L12
     FILE 'CAOLD' ENTERED AT 17:25:37 ON 14 MAR 2001
             0 S L9
L13
---Logging off of STN---
Executing the logoff script...
=> LOG Y
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COST IN U.S. DOLLARS	SINCE FILE :ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.31	303.15
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-4.48

STN INTERNATIONAL LOGOFF AT 17:26:03 ON 14 MAR 2001